

Electronic Structure Fermi Liquid Theory of High T_c Superconductors; Comparison with Experiments*

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The most exciting issues in the microscopic theory of high T_c superconductivity are embodied in the questions: "What are the mechanisms of high T_c ?" and "What is the nature of the normal state of the Cu-oxide superconductors?" In particular, a major issue in understanding of the normal state of these systems is how well a Fermi liquid picture (e.g., LDA energy band theory) works in describing their normal state properties.

For years, there has been controversy and confusion among theorists as well as experimentalists on whether the 'normal' state of the Cu-oxide superconductors is a Fermi liquid or some other exotic ground state. However, some experimentalists (including Arko *et al.*) are clarifying the nature of the normal state of the high T_c superconductors by surmounting the experimental difficulties in producing clean, well-characterized surfaces so as to obtain meaningful high-resolution angle-resolved photoemission data, which agrees with earlier positron-annihilation experiments by Smedskjaer *et al.* The experimental work on high-resolution angle-resolved photoemission by Campuzano *et al.* and positron-annihilation studies by Smedskjaer *et al.* has verified our calculated Fermi surfaces in $\text{YBa}_2\text{Cu}_3\text{O}_7$ superconductors and has provided evidence for the validity of our energy band approach. Similar good agreement has been found for $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ by Olson *et al.*

In addition, LDA predictions on the normal state transport properties for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_7$ by Allen *et al.* are qualitatively in agreement with experiments on single crystals. Moreover, the measured Hall coefficient for the non-Cu based $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ system was found to be negative, which agrees with our energy band calculation. Recently, for $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ systems, we obtained (together with Hamada and Massidda) a positive Hall coefficient for the magnetic field oriented perpendicular to the Cu-O planes. This is to be compared with a negative experimental value found for $x < 0.18$ and recent experiments which show a change of sign of this Hall coefficient (from negative to positive with increasing x) for $x = 0.18$. These results on Hall coefficients indicate a trend (previously found for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$) toward a regime where the conventional band theoretical description comes into better agreement with experiment.

As a Fermi liquid (metallic) nature of the 'normal' state of the high T_c superconductors becomes evident, these experimental observations have served to confirm the predictions of our local density functional calculations and hence the energy band approach as a valid natural starting point for further studies of their superconductivity.

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